Possible polaron manifestation in cobalt XAS of cobalt-doped TiO₂

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Ample enthusiasm and a measure of mystery and controversy have surrounded cobalt-doped TiO₂ since its discovery as a room temperature ferromagnetic semiconductor. One of the outstanding questions pertains to the unresolved mechanism mediating ferromagnetism in those materials. One mechanism proposed by Kaminski and Das Sarma (2002), which was recently applied specifically to doped oxides by Coey et al. (2005), is based on polaron percolation. Our studies of various cobalt-doped titanium oxides have revealed a surprising new spectral feature in x-ray absorption spectroscopy for Co doping levels below 2%. Based on our observations, the feature appears to be intimately related to the polarons of the polaron percolation theory. We independently deduced a percolating defect picture that qualitatively agrees with the polaron percolation theory. Furthermore, based on Monte Carlo simulations with a hard sphere approximation, the defect size is determined to be 6 Å. The same effective hard sphere radius can be deduced from Coey's analysis for impurity band delocalization.

While the ferromagnetism is percolation driven, the spectral feature we observe is related to isolated polarons (and substitutional cobalt atoms). We correspondingly observe a decline of the spectral feature that coincides with the increasing magnetic moment with increasing polaron concentration. This fascinating manifestation and its significant substantiation of important features of the polaron percolation model may help to finally resolve the issue of ferromagnetism in magnetically doped oxides.